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Cubic to cubic phase transition in $(NH_4)_3SnF_7$ ferroelastic crystal – Raman scattering study

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Binary salt of $(NH_4)_2SnF_6 \bullet NH_4F$ has been synthesized and crystallized by a special procedure of solvent crystallization providing high quality single crystal samples used for optical vibrational spectroscopy.

Detailed Raman scattering and infrared absorption in a wide temperature range confirmed phase transition in $(NH_4)_2SnF_6 \bullet NH_4F$ at 360 K. Earlier this phase transition was found to be between two cubic phases (Pa-3↔Pm-3m) [1].

Wide band was found in the Raman spectra at 600 cm^{-1}, that corresponds to the full symmetry stretching mode $\nu_1(A_{1g})$ of octahedric SnF_6 groups. Under cooling it splits into a doublet at 586 cm^{-1} of the $(Sn2)F_6$ group and at 580 cm^{-1} – of the $(Sn1)F_6$ one. Internal bending vibrations $\nu_2(Eg)$ of SnF_6 groups were found at 470 cm^{-1}. Strong peak near 246 cm^{-1} is formed by two coinciding bending $\nu_5(F_{2g})$ modes of $(Sn2)F_6$ и $(Sn1)F_6$ octahedrons. Rotating modes of SnF_6 groups are found at 67 cm^{-1} and 87 cm^{-1}. Cooling down to 8 K results in slight displacements of these lines and activates several new ones. In particular new lines appear at 160 cm^{-1} and 25 cm^{-1} below 200 K but their temperature dependences do not look like of a soft mode but rather like being induced some relaxations typical for ordering processes.

All Raman active internal bending modes $\nu_2(E)$ and $\nu_4(F2)$ of NH_4 ions are observed in the *Pa*-3 phase though being rather wide, and cooling down to 8 K activates up to 10 peaks at least. Spectral band of NH_4 internal stretching at 3000-3350 cm^{-1} is rather asymmetrical and may be deconvolved into four lines at least; under cooling down to 8 K it splits into six separated peaks.

All observed transformations of the Raman spectra are quite typical for ordering processes both SnF_6 and NH_4 groups below transition from the *Pm*-3*m* phase to the *Pa*-3 one.

Besides these spectral transformations formation of some thin films was observed at the sample surface that did not produce traceable Raman signal and did not look like destruction of the binary salt in the bulk.

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1. I.N. Flerov, M.S. Molokeev, N.M. Laptash, A.A. Udovenko, E.I. Pogoreltsev, S.V. Mel'nikova, S.V. Misyul, *J. Fluor. Chem.* **178**, 86 (2015).